ENERGY LANDSCAPES, SCALE-FREE NETWORKS AND APOLLONIAN PACKINGS

JONATHAN P. K. DOYE AND CLAIRE P. MASSEN

University Chemical Laboratory, Lensfield Road, Cambridge CB2 1EW, United Kingdom

We review recent results on the topological properties of two spatial scale-free networks, the inherent structure and Apollonian networks. The similarities between these two types of network suggest an explanation for the scale-free character of the inherent structure networks. Namely, that the energy landscape can be viewed as a fractal packing of basins of attraction.

1. Introduction

The potential energy as a function of the coordinates of all the atoms in a system defines a multi-dimensional surface that is commonly known as an energy landscape.[1] Characterizing such energy landscapes has become an increasingly popular approach to study the behaviour of complex systems, such as the folding of a protein[2] or the properties of supercooled liquids.[3,4] The aim is to answer such questions as, what features of the energy landscape differentiate those polypeptides that are able to fold from those that get stuck in the morass of possible conformations, or those liquids that show super-Arrhenius dynamics ('fragile' liquids) from those that are merely Arrhenius ('strong' liquids).

Such approaches have to be able to cope with the complexity of the potential energy landscape—for example, the number of minima is typically an exponential function of the number of atoms.[5] One such approach is the inherent structure mapping pioneered by Stillinger and coworkers.[6] In this mapping each point in configuration space is associated with the minimum obtained by following the steepest-descent pathway from that point. Thus, configuration space is partitioned into a set of basins of attraction surrounding the potential energy minima, as illustrated in Fig. 1.

One of the original aims of this approach was to remove the vibrational motion from configurations generated in simulations of liquids to give a clearer picture of the underlying 'inherent structure', hence the common name for the mapping. Of more interest to us is that it breaks the energy landscape down into more manageable chunks, whose properties can be more easily established and understood. As an example of the utility of this approach, the classical partition function can be expressed as an integral over the whole of configuration space, but performing this integral (except numerically through say Monte Carlo) is nigh impossible, because
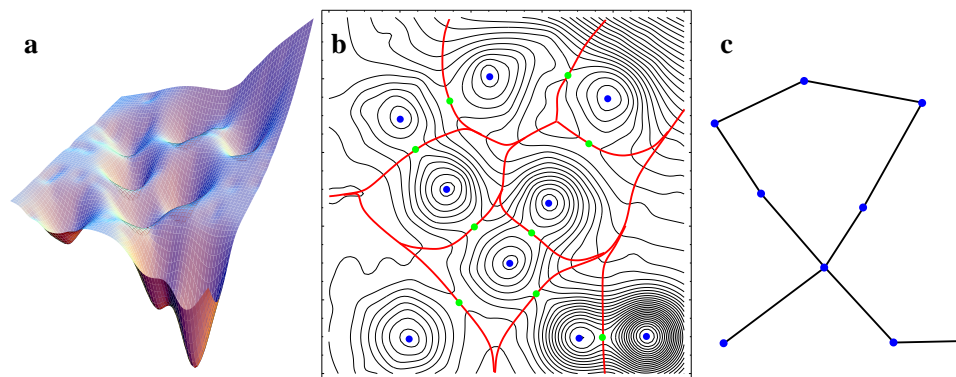
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Figure 1.   (a) A model two-dimensional potential energy surface, (b) the contour plot of this surface showing the 'inherent structure' division of the energy landscape into basins of attraction (the minima and transition states are represented by points and the basin boundaries by the thick lines), and (c) the representation of the landscape as a network.

of the complexity of the potential energy landscape. However, if this integral is divided up into separate integrals over each basin of attraction, analytical approximations to these individual integrals can easily be obtained by assuming that the basins can be modelled as a harmonic well surrounding the minimum at the centre of the basin. Calculation of an approximate partition function, then just reduces to a characterization of the properties of the potential energy minima and their associated basins.[7] As well as providing insights into the contributions of different regions of the energy landscape to the thermodynamics, quantitative accuracy can be obtained when account is taken of the anharmonicity of the basins.[8]

Similarly, an energy landscape perspective on the dynamics can be formulated in terms of the transitions between the basins of attraction. Except at sufficiently high temperature, a trajectory of a system can be represented as a series of episodes of vibrational motion within a basin, punctuated by occasional hopping between basins along a transition state valley.[9] In a coarse-grained view that ignores the vibrational motion, the dynamics is a walk on a network where the nodes correspond to minima and there are edges between minima that are directly connected by a transition state.[a] An example of such an 'inherent structure' network is also illustrated in Fig. 1.

Although there has been much work characterizing energy landscapes with the aim of gaining insights into particular systems, some of the fundamental properties of such landscapes, particularly those related to their global structure and organization, have received relatively little attention. For example, what is the nature of

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[a]By a transition state we mean a stationary point on the potential energy landscape that has one eigendirection with negative curvature. The steepest-descent pathways from the transition state parallel and anti-parallel to this Hessian eigenvector then provide a unique definition of the two minima connected by this transition state.
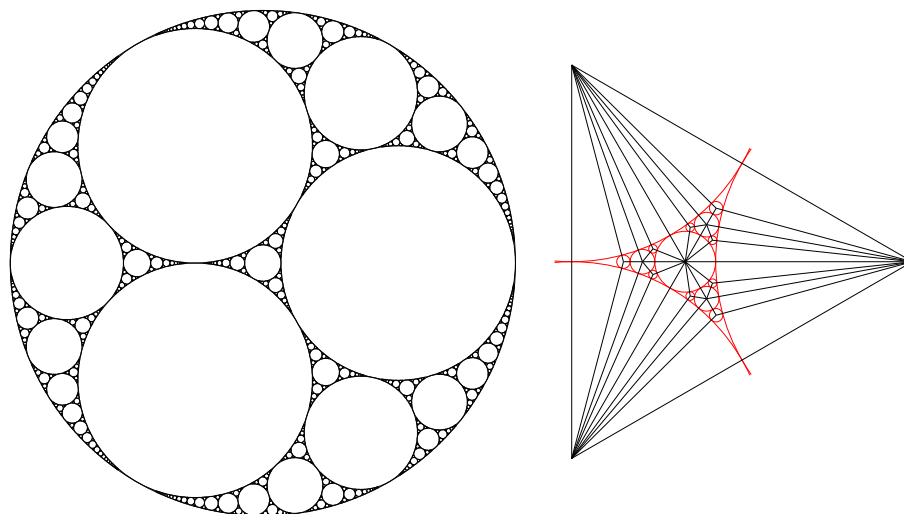
Figure 2.   The Apollonian packing of a circle, and the corresponding network for the central interstice between the initial disks after three generations of disks have been added.

the division of the energy landscape into basins of attraction and does the inherent structure network have a universal form? In this chapter, we will be reviewing recent results that address exactly these questions. The system that we will be analysing is a series of small Lennard-Jones (LJ) clusters for which the complete inherent structure network can be found.

Another approach to understanding the properties of complex systems that has received much attention recently is through an analysis of the system in terms of networks.[10,11] The systems analysed in this way have spanned an impressive range of fields, including astrophysics,[12] geophysics,[13] information technology,[14] biochemistry,[15,16] ecology,[17] and sociology.[18] Initially, the focus was on relatively basic topological properties of these networks, such as the average separation between nodes and the clustering coefficient to test whether they behaved like the Watts-Strogatz small-world networks,[19] or the degree distribution[b] to see if they could be classified as scale-free networks.[20]

To summarize our recent results we found that the inherent structure networks associated with the LJ clusters behaved as fairly typical scale-free networks.[21,22,23] However, the origins of most scale-free networks can be explained in terms of network growth models, where there is preferential attachment to nodes with high degree during network growth.[20] By contrast, the inherent structure networks are static. They are determined just by the potential describing the interatomic interactions and the number of atoms in the system. So, why are they scale free?

One of the important features of the inherent structure networks is their embed-

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[b]In network parlance, the degree k is the number of connections to a node.
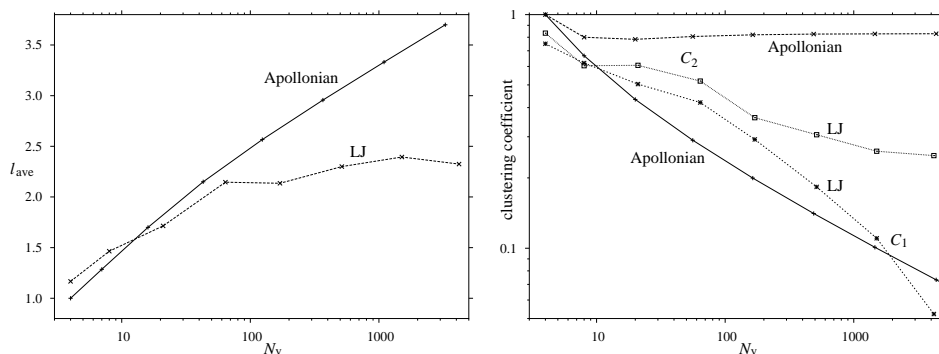
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Figure 3.   The scaling of the average separation between nodes and the clustering coefficient with network size for LJ clusters with 7 to 14 atoms, and two-dimensional Apollonian networks with increasing numbers of generations.

ding in configuration space. There have been a number of model spatial scale-free networks proposed,[24,25,26,27] but the ones on which we wish to focus are Apollonian networks.[28,29] These networks are associated with Apollonian packings, an example of which is given in Fig. 2. To generate such a packing, one starts with a set of touching disks (or hyperspheres if one is interested in higher-dimensional packings) and then to each interstice in the packing, new disks are added that touch each disk surrounding the interstice. At each subsequent generation the same procedure of adding disks to the remaining interstices is applied. The complete space-filling packing is obtained by repeating this process *ad infinitum*. The Apollonian network is then the contact network between adjacent disks (Fig. 2).

One of the reasons that the Apollonian network provides a useful comparison to the inherent structure networks is that spatial regions (the disks) are automatically associated with each node in the network, which is somewhat similar to the association of the basins of attraction with the minima on an energy landscape. Furthermore, in both networks edges are based on contacts between those spatial regions that are adjacent. As a consequence, for two-dimensional examples, both types of network are planar, that is, they can be represented on a plane without any edges crossing.[30] This feature contrasts with the other model spatial scale-free networks.[24,25,26,27] Therefore, in this chapter we will be comparing the properties of the inherent structure and Apollonian networks.

2. Comparing Apollonian and inherent structure networks

We were able to obtain the complete inherent structure networks for all LJ clusters with up to 14 atoms. For the largest cluster, the network had 4196 nodes and 87 219 edges. By contrast, the Apollonian networks have an infinite number of nodes. Therefore, to allow a comparison we consider finite Apollonian networks obtained by only considering the first t generations of disks. The comparison we make is usually between the LJ_{14} network and a two-dimensional Apollonian network with a similar
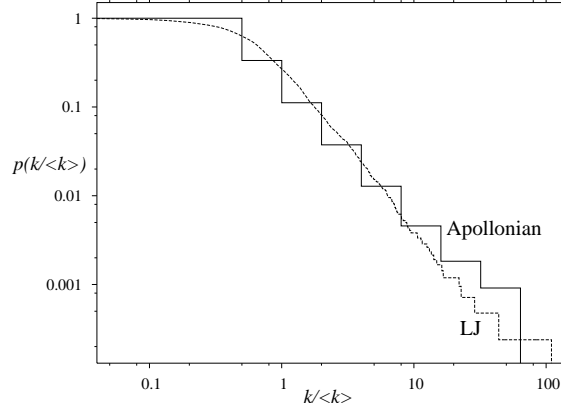
Figure 4.   The cumulative degree distributions for the inherent structure and Apollonian networks.

number of nodes (in fact with $t = 7$ and 4376 nodes and 13 122 edges). One could argue that it would be more appropriate to compare to an Apollonian network with the same spatial dimension. However, the properties of the Apollonian networks are very similar irrespective of dimension, so we chose to use the two-dimensional example simply because the properties of this case have been most comprehensively worked out.

To study the size dependence of the network properties, as in Fig. 3 we have to make a further choice. For the inherent structure networks we follow clusters with an increasing number of atoms, and hence an increasing dimension of configuration space. Again it could be argued that we should be comparing to an Apolonian network of fixed number of generations, but increasing dimension, but the useful feature of examining a network of fixed dimension and increasing t instead is that the variable t behaves in a somewhat similar way to the number of atoms. For example, the number of nodes is an exponential function of t, whereas it only increases polynomially with the dimension of the system.[29] As already mentioned, the number of minima is an exponential function of the number of atoms.

From Fig. 3, one can see that both types of networks have small-world properties. Firstly, for both networks the average separation between nodes scales no more than logarithmically with system size, as for a random graph. The stronger sub-logarithmic behaviour for the inherent structure networks is because the average degree increases with network size (the random graph result is in fact $l_{\mathrm{ave}} = \log N_v / \log\langle k\rangle$) whereas it is approximately constant for the Apollonian networks. The increase in $\langle k\rangle$ is simply because the ratio of the number of transition states to minima on a potential energy landscape is a linear function of the number of atoms.[31] Secondly, the clustering coefficient, one measure of the local ordering within a network, has values that are significantly larger than for a random network. The size dependence of this property depends on how it is defined. If it is
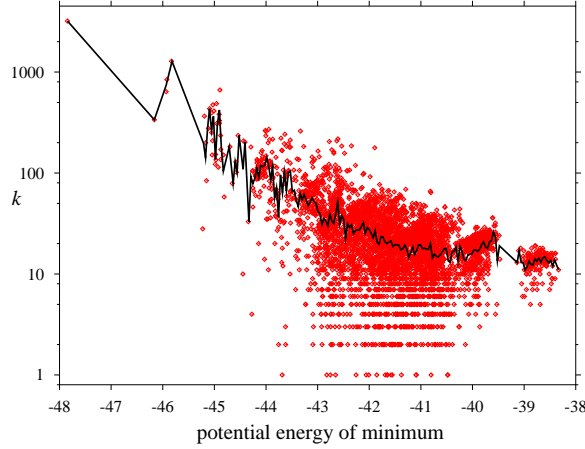
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Figure 5.   The dependence of the degree of a node on the potential energy of the corresponding minimum for LJ_{14}. The data points are for each individual minimum and the solid line is a binned average.

as the probability that any pair of nodes with a common neighbour are themselves connected (C_1) then it decreases quite rapidly with size. The second definition (C_2) is as the average of the local clustering coefficient, where the latter is defined as the probability that the neighbours of a particular node are themselves connected. The second definition gives more weight to the low-degree nodes that, as we shall see later, have a higher local clustering coefficient. That C_2 tends to a constant value for the Apollonian network, rather than decaying weakly as for the inherent structure networks, reflects the stronger degree dependence of the local clustering coefficient.

Both networks also have a power-law tail to their degree distribution, and so are scale-free networks. The exponent is slightly larger for the inherent structure networks (2.78 compared to 2.59). This heterogeneous degree distribution is easier to understand for the Apollonian network, and reflects the fractal nature of the packings.[32] At each stage in the generation of the network, the degrees of the nodes double, i.e. new nodes preferentially connect to those with higher degree, and so the highest degree nodes correspond to those that are 'oldest' and have larger associated disks.

For the inherent structure networks, the high-degree nodes correspond to minima with low potential energy (Fig. 5). Our rationale for this correlation between degree and potential energy is that the lower-energy minima have larger basin areas,[33] and hence longer basin boundaries with more transition states on them. The scale-free character of these networks must reflect the hierarchical packing of these basins with larger basins surrounded by smaller basins, which in turn are surrounded by smaller basins, and so on, in a manner somewhat similar to the Apollonian packing. Thus, the comparison of the inherent structure and Apollonian networks can provide some
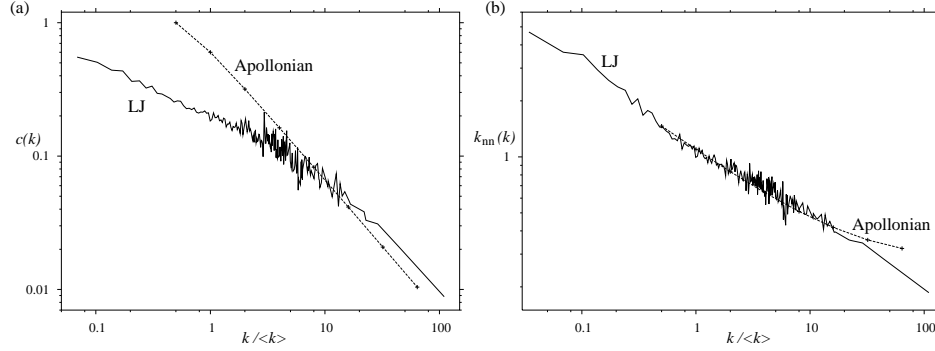
Figure 6.   The degree dependence of (a) the local clustering coefficient and (b) k_{nn}, the average degree of the neighbours of a node for the inherent structure and Apollonian networks. Both lines represent the average values for a given k.

check of the plausibility of this potential origin of the scale-free behaviour of the inherent structure networks.

Figure 6 shows that the two types of networks also behave similarly when we look at more detailed properties of the networks. Both have a local clustering coefficient that decreases strongly with increasing degree. For the Apollonian network, it is actually inversely proportional to the degree[29] — a feature that has been previously seen for other deterministic scale-free networks[34,35,36] and that has been interpreted in terms of a hierarchical structure to the network[35,37] — whereas for the inherent structure networks the degree dependence is somewhat reduced at small k. This similar behaviour partly reflects the common spatial character of the networks. The smaller low-degree nodes have a more localized character and so their neighbours are more likely to be connected, whereas the larger high-degree nodes can connect nodes that are spatially distant from each other and so are less likely to be connected.

The behaviour of $c(k)$ also partly reflects the correlations[38] evident in Fig. 6(b). Both networks are disassortative, that is nodes are more likely to be connected to nodes with dissimilar degree. By contrast, for an uncorrelated network, $k_{nn}(k)$ would be independent of degree. However, it is well known that disassortativity can arise for networks, as here, in which multiple edges and self-connections are not present.[39] Indeed, for the inherent structure networks $k_{nn}(k)$ for a random network with the same degree distribution looks almost identical.[22] An additional source of disassortativity is present in the Apollonian networks, because, except for the initial disks, there are no edges whatsoever between nodes with the same degree; disks created in the same generation all go in separate interstices in the structure and so cannot be connected. Therefore, that $k_{nn}(k)$ for the two types of networks follow each other quite so closely is probably somewhat accidental.

The behaviour seen for most of the network properties discussed so far is fairly common for scale-free networks. Therefore, a better test of the applicability of the
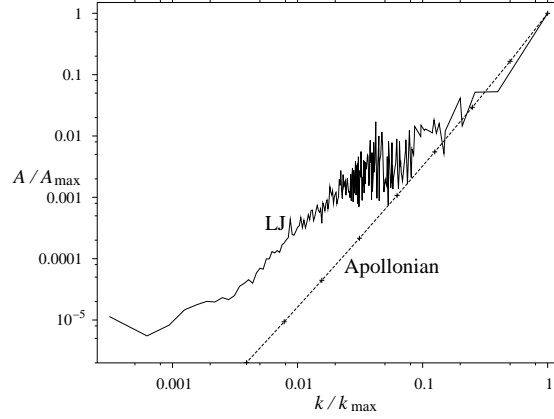
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Figure 7.   The degree dependence of the basin areas for the LJ_{14} energy landscape and disk areas for the Apollonian packing. Both lines represent the average values for a given k.

Apollonian analogy to the energy landscape is to examine the spatial properties of the two systems directly. For the inherent structure networks, in agreement with the suggestion made earlier, there is a strong correlation between the degree of a node and the hyperarea of the basin of attraction that is similar to the degree dependence of the disk area seen for the Apollonian networks (Fig. 7). This result therefore implies that there is also a strong dependence of the basin area on the energy of a minimum with the low-energy minima having the largest basins. It also provides strong evidence that the scale-free topology of the inherent structure networks reflects the heterogeneous distribution of basin areas.

The distribution of disk areas for the Apollonian packing reflects its fractal character.[32] It is in fact a power-law[40] with an exponent that depends upon the fractal dimension of the packing,[41] as illustrated in Fig. 8 For high-dimensional packings this exponent tends to -2.[29] Preliminary results suggest that there is a similar power-law distribution for the hyperareas of the basins of attraction on an energy landscape, confirming the deep similarity between these two types of system, and suggesting that configuration space is covered by a fractal packing of the basins of attraction.

3. Conclusion

In this chapter we have looked at some of the fundamental organizing principles of complex multi-dimensional energy landscapes. By viewing the landscapes as a network of minima that are linked by transition states, we have found that the topology of this network is scale-free. Unlike most scale-free networks, the origin of this topology must be static. We believe that it is driven by a very heterogeneous size distribution for the basins of attraction associated with the minima, with the large basins having many connections. In this paper, we have explored whether space-filling packings of disks and hyperspheres, such as the Apollonian packings,
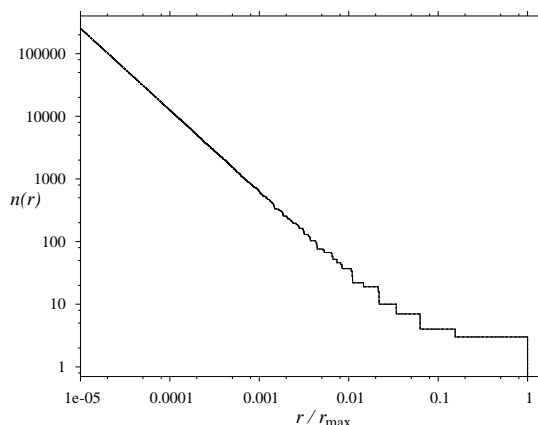
Figure 8.   The cumulative distribution for disks with radius greater than r in a two-dimensional Apollonian packing.

and their associated contact networks can provide a good model of how the energy landscape is organized. We have shown that these systems share a deep similarity both in the topological properties of the networks and the spatial properties of the packings. In fact, our results suggest that the energy landscape can be viewed as a fractal packing of basins of attraction. Although this conclusion can provide an explanation for the scale-free topology of the inherent structure network, it itself demands an explanation. Why are the basins of attraction organized in this fractal manner? We will explore this in future work.

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